Propulsion Chemistry for CFD Applications

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In order to perform combustion analyses for advanced propulsion systems, the thermodynamic properties of the fuel, oxidizer, and all significant combustion products must be available. Conventional hydrocarbon propellants, such as RP–1, pose a difficult challenge because of the many species which are involved. Even small amounts of soot which can be formed cause severe heating and surface deposition problems. Data for many species are already available in literature, but many are not. Most of the data are for low pressure only (ideal gases). SECA, Inc. has developed a real fluids model for generating thermal and caloric equations of state and predicting transport properties suitable for direct use in computational fluid dynamics (CFD) analyses of finite-rate combustion processes. Prior to the advent of CFD design methodology, experimental property values alone were used for design purposes.

SECA's real fluids model utilizes ideal gas properties as a basis upon which dense gas, liquid, and multi-phase effects are added to cover the entire range of propellant properties. The individual correction equations have been carefully selected to provide highly accurate predictions over a wide range of conditions while requiring a minimum of information for the individual species. The multitude of experimental data and previous estimation techniques available in the literature substantiate this procedure for producing accurate estimates of properties for well defined mixtures of pure species.

When applied to actual fuels, such as RP–1, additional complications must be considered. RP–1 is compromised of literally hundreds of species, which vary in quality from lot to lot of fuel. SECA has purchased chemical analyses of RP–1 samples (since such data were not found in the literature) to provide a representative set of species which comprise this fuel. These species were then represented by a surrogate which matched species type and molecular size with a modest number of neat hydrocarbons. The RP–1 surrogate was then simulated with the real fluids code. The results predicted with the thermal equation of state are presented in figure 58. This simulation provides not only accurate thermodynamic properties, but also realistic species for subsequent estimation of combustion kinetics, including soot formation and oxidation.

Applications of the real fluids model to the analyses of advanced launch systems are in progress. Future applications to JP and diesel type fuels and pulverized coal combustion are envisioned. The real fluids model may be used as a subroutine in a CFD code, as a stand-alone code to predict fluid properties, or as a means to provide tabulated thermodynamic and transport property data for convenient use.

The thermodynamic property routines developed in this investigation allow accurate prediction of combustion processes under a wide range of operating conditions and for the propellants expected to be used in the advanced launch vehicles now being designed. The use of these property routines with CFD design methodology will result in more economical and timely designs.

Sponsor: SECA, Inc., Huntsville, AL

Biographical Sketch: Kevin Tucker is currently a member of the computational analysis team in the Fluid Dynamics Analysis branch. He received his M.S. degree from the University of Alabama in Huntsville in 1992. His recent work is focused on application of CFD methods for rocket engine combustion devices.

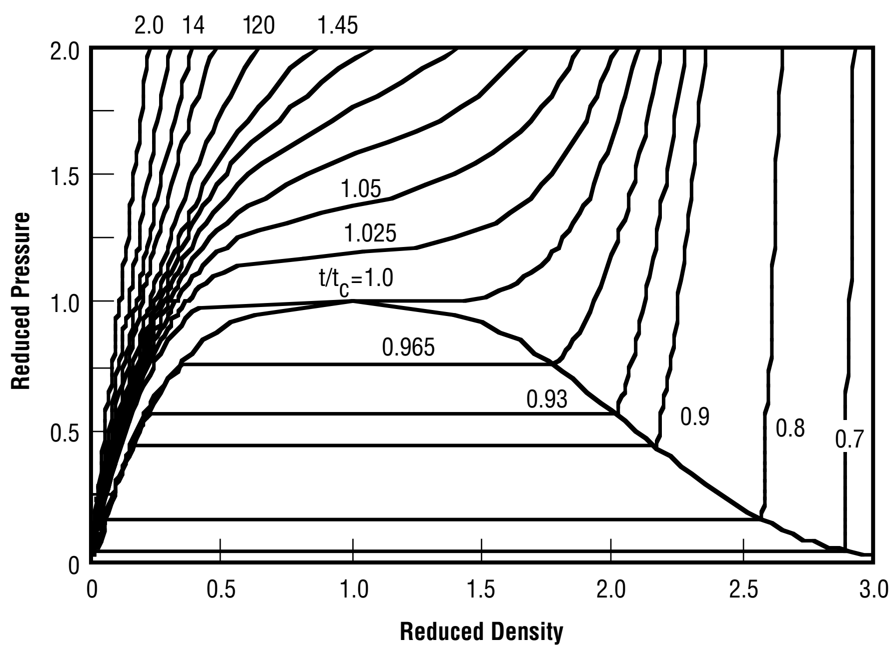

FIGURE 58.—RP–1 thermal equation of state predictions.